SOLVENT, TEMPERATURE And CONCENTRATION EFFECTS On THE OPTICAL ACTIVITY Of CHIRAL FIVE-And-SIX MEMBERED RING KETONES CONFORMERS

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Chiral five-and-six membered ring ketones are important molecules that are found in many biological systems and can exist in many possible conformers. In this talk, experimental and computational investigation of solvent, temperature and concentration effects on the circular dichroism (CD) and optical rotation (OR) of (R)-3 -methylcyclohexanone (R3MCH), (R)-3-methylcyclopentanone (R3MCP) and carvone conformers will be discussed. CD and OR measurements of these ketones gaseous samples and in ten common solvents of wide polarity range for different concentrations and sample temperatures were recorded and related to molecular conformation. Density functional theoretical calculations were performed using Gaussian09 at B3LYP functions with aug-cc-pVDZ level of theory. Also, CD and OR spectra for the optimized geometries of the ketones dominant conformers were computed over the ultraviolet and visible region in the gas phase as well as in ten solvents of varying polarity range, and under the umbrella of the polarizable continuum model (PCM). By comparing theoretical and experimental results, few thermodynamic parameters were deduced for the individual equatorial and axial conformers of each molecule in gas phase and in solvation.